Indian J. Phys. 49, 49–53 (1975)

On the relativistic electronic states of a diatomic one-dimensional lattice

N. D. Sen Gupta

Tata Institute of Fundamental Research, Bombay 400005

(*Received* 2 *September* 1974)

The relation between the energy and momentum of an electron in a linear array of δ-function potentials obeying the Dirac equation for a diatomic lattice is obtained.

1. Introduction

Recently Subramanian & Bhagwat (1971, 1972) have obtained the relation between the energy and momentum of an electron in a linear array of δ-function potential for a monatomic lattice, obeying the Dirac equation with the help of the transfer matrix introduced by Saxon & Hunter (1949), and Luttinger (1951). The object of this short paper is to extend the investigation to the case of a diatomic lattice, following a similar method. The linear array of δ-function potentials for a diatomic lattice is described by

$$V(x) = \hbar c \sum_{-\infty}^{\infty} \{\zeta_1 \delta(x-na)+\zeta_2\delta(x+\frac{a}{2}-na)\}, \quad \ldots \quad (1)$$

ζ_1 and ζ_2 are dimensionless quantities which determine strengths of the sources, a is the lattice distance.

The next section is a very brief prelude to the construction of transfer matrices relevant to the problem, so that the calculations for the dispersion relation are much simplified. The desired dispersion relation for a diatomic lattice is obtained in section 3. The last section is devoted to a short discussion of the result obtained.

2. The One-dimensional Dirac Equation with a δ-Function Potential

Let us consider a δ-function potential at x_0 of strength ζ_0, so that the time-independent one dimensional Dirac equation is given by

$$\left(\frac{E}{c}+i\hbar c\alpha \frac{d}{dx}+\beta mc \right) \Psi(x) = \zeta_0\hbar\delta(x-x_0)\psi(x). \quad (2)$$

The subscript is redundant as only one α appears. $\Psi(x)$ is discontinuous at $x = x_0$. In order to obtain the discontinuity one notes that

$$i\frac{d}{du}\{\Psi(x_0+u)-\Psi(x_0-u)\} = \zeta_0\delta(u)\{\Psi(x_0+u)+\Psi(x_0-u)\}. \qquad \ldots \quad (3)$$

Integrating between the limits $(u, -u)$ and passing to the limit $u \to 0$, one obtains

$$\Psi(x_0+0)-\Psi(x_0-0) = -i\frac{\zeta_0}{2}\alpha\{\Psi(x_0+0)+\Psi(x_0-0)\}, \qquad (4)$$

so that

$$\Psi(x_0+0) = \exp(-i2\alpha\phi_0).\Psi(x_0-0), \quad \tan\phi_j = \frac{\zeta_j}{2}. \qquad (5)$$

The most general solution of eq. (2) for $x \neq x_0$ may be written as

$$\Psi(x) = (1-e^{-\theta}\beta)(\exp(i\epsilon x).\boldsymbol{u}+\exp(-i\epsilon x).\beta\boldsymbol{v}), \qquad (6)$$

where $\boldsymbol{u}$ and $\boldsymbol{v}$ are arbitrary spinors, such that

$$\alpha\boldsymbol{u} = \boldsymbol{u} \quad \text{and} \quad \alpha\boldsymbol{v} = \boldsymbol{v}; \qquad (7)$$

$$e^{\theta} = \frac{mc^2}{E-c\hbar\epsilon} = \frac{E+c\hbar\epsilon}{mc^2}, \quad \epsilon = +\frac{1}{\hbar c}(E^2-m^2c^4)^{\frac{1}{2}}. \qquad (8)$$

The effect of the discontinuity at x_0 is to introduce a transformation of the spinors $(\boldsymbol{u}_-(x_0))$, $\boldsymbol{v}_-(x_0)$ to $(\boldsymbol{u}_+(x_0))$, $(\boldsymbol{v}_+(x_0))$, such that

$$\Psi(x_0\pm0) = (1-e^{-\theta}\beta)\{\exp(i\epsilon x_0).\boldsymbol{u}_\pm(x_0)+\beta\exp(-i\epsilon x_0).\boldsymbol{v}_\pm(x_0)\}. \qquad \ldots \quad (9)$$

From eq. (5), it follows that

$$(1-\sigma_1e^{-\theta})\exp(i\epsilon x_0\sigma_3).U_+(x_0) = \exp(-i2\phi_0\sigma_3)(1-\sigma_1e^{-\theta})\exp(i\epsilon x_0\sigma_3).U_-(x_0). \qquad \ldots \quad (10)$$

$U_\pm$ are column vectors with elements $(\boldsymbol{u}_\pm, \boldsymbol{v}_\pm)$, and σ_1, σ_2, which operate on them are given by

$$\sigma_1 = \begin{vmatrix} 0, & 1 \\ 1, & 0 \end{vmatrix} \qquad \sigma_2 = \begin{vmatrix} 1, & 0 \\ 0, & -1 \end{vmatrix}. \qquad \ldots \quad (11)$$

Next, a continuous change from x_1 to x_2 leads to

$$U_-(x_2) = \exp(i\epsilon(x_2-x_1)\sigma_3).U_+(x_1). \qquad \ldots \quad (12)$$

Any one of those transformations, say Λ, or any finite number of products of similar transformation satisfy the condition

$$\tilde{\Lambda}\sigma_3\Lambda = \sigma_3 \quad \text{and} \quad \Lambda^* = \sigma_1\Lambda\sigma_1; \qquad \ldots \quad (13)$$

'$\sim$' stands for hermitian conjugate. This is a consequence of the fact that $\tilde{\Psi}\alpha\psi$ is constant and hence

$$\tilde{\boldsymbol{u}}\cdot\boldsymbol{u}-\tilde{\boldsymbol{v}}\cdot\boldsymbol{v} = \text{constant}. \qquad \ldots \quad (14)$$

It is easy to see that such a Λ has eigen values either $(e^{\lambda}, e^{-\lambda})$ or $(e^{i\mu}, e^{-i\mu})$, with λ and μ real.

3. The Transfer Matrix and the Dispersion Relation

We can now easily construct a representation of the transfer matrix in the space of $(\boldsymbol{u}, \boldsymbol{v})$, for the problem with potential V of eq. (1).

(a) (i) Let us start from -0 the transformation due to the passage of discontinuity at 0 is given by

$$U_{+}(0) = \frac{1}{1-e^{-2\theta}}(1+\sigma_1 e^{-\theta})\exp(-i2\phi_1\sigma_3).(1-\sigma_1 e^{-\theta})U_{-}(0). \qquad \ldots \quad (15)$$

(ii) The wave function continuously changes from $+0$ to $a/2-0$, thus eq. (12) leads to,

$$U_{-}\left(\frac{a}{2}\right) = \exp\left(i\epsilon\frac{a}{2}\sigma_3\right).U_{+}(0). \qquad \ldots \quad (16)$$

(iii) Next, it passes over the discontinuity at $a/2$ and from eq. (10) the transformation is given by

$$U_{+}\left(\frac{a}{2}\right) = \frac{1}{1-e^{-2\theta}}(1+\sigma_1 e^{-\theta})\exp(-i2\phi_2\sigma_3).(1-\sigma_1 e^{-\theta})U_{-}\left(\frac{a}{2}\right). \qquad \ldots \quad (17)$$

(iv) Finally, the wave function continuously changes from $(a/2)+0$ to $a-0$, so that

$$U_{-}(a) = \exp\left(i\epsilon\frac{a}{2}\sigma_3\right).U_{+}\left(\frac{a}{2}\right). \qquad \ldots \quad (18)$$

(b) The complete transfer matrix is thus obtained as

$$U_{-}(a) = \Sigma_2\Sigma_1 U_{+}(0), \qquad \ldots \quad (19)$$

where

$$\Sigma_j = -\frac{\exp\left(i\epsilon\frac{a}{2}\sigma_3\right)}{1-e^{-2\theta}}(1+\sigma_1 e^{-\theta})\exp(-i2\phi_j\sigma_3).(1-\sigma_1 e^{-\theta}). \qquad \ldots \quad (20)$$

Now, since $V(x)$, (eq. (1)) is periodic, Floquet's theorem states that it is possible to construct solutions such that

$$U_{-}(a) = \exp(iKa).U_{-}(0), \qquad \ldots \quad (21)$$

thus $U_{-}(0)$ is an eigen vector of the transfer matrix.

Further, allowed energy states corresponds to K real. It has already been noted that the transfer matrix $\Sigma_2\Sigma_1$ has eigenvalues of the from $\exp(iKa)$, (K either real or imaginary) hence for allowed energies

$$\text{tr}.\Sigma_2\Sigma_1 = 2\cos ka, \qquad \dots \quad (22)$$

(k real). Since $\Sigma_2\Sigma_1$ is written in terms of σ_1, σ_3 it is easy to find the trace, as terms which contain σ_1 and σ_3 as linear factors do not contribute.

$$\begin{aligned}\tfrac{1}{2}\text{tr}.\Sigma_2\Sigma_1 = {} & \cos a\epsilon \cos 2\phi_1 \cos 2\phi_2 + \sin a\epsilon \cosh\theta \sin 2(\phi_1+\phi_2) \\ & -\sin 2\phi_1 \sin 2\phi_2(\cosh^2\theta \cos a\epsilon - \sinh^2\theta). \qquad \dots \quad (23)\end{aligned}$$

Expressing ϕ_1, ϕ_2 in terms of ζ_1, ζ_2, we obtain finally the desired dispersion relation,

$$\begin{aligned}\left(1+\frac{\zeta_1^2}{4}\right)\left(1+\frac{\zeta_2^2}{4}\right)\cos ak = {} & (\zeta_1+\zeta_2)\left(1-\frac{\zeta_1\zeta_2}{4}\right)\cosh\theta \sin a\epsilon \\ & +\zeta_1\zeta_2\left(\cosh 2\theta \sin^2\frac{a\epsilon}{2} - \cos^2\frac{a\epsilon}{2}\right) + \left(1-\frac{\zeta_1^2}{4}\right)\left(1-\frac{\zeta_2^2}{4}\right)\cos a\epsilon. \quad \dots \quad (24)\end{aligned}$$

4. Discussion

The above dispersion relation agrees with that of Saxon & Hunter (1949) for the non-relativistic case, when terms in second and higher orders in ζ_1 and ζ_2 which depend on strengths of the potentials, are neglected. Further, this dispersion relation, reduces to that of a monatomic lattice obtained for the first time by Subramanian & Bhagwat (1971) and later obtained by Fairbairn *et al* (1973), if either $\zeta_2 = 0$ and $\zeta_1 = \zeta$ or $\zeta_1 = 0$ and $\zeta_2 = \zeta$.

In order to examine the case when the strengths are nearly equal, relation (24) is written in the form

$$\begin{aligned}S_+\left(k, \frac{\zeta_1+\zeta_2}{2}, \frac{a}{2}\right) S_-\left(k, \frac{\zeta_1+\zeta_2}{2}, \frac{a}{2}\right) = {} & \frac{(\zeta_1-\zeta_2)^2}{8}\Big\{\sin^2\frac{ak}{2} - \cosh 2\theta \sin^2\frac{a\epsilon}{2} \\ & + \frac{1}{4}(\zeta_1+\zeta_2)\cosh\theta \sin a\epsilon + \frac{1}{64}(\zeta_1^2+6\zeta_1\zeta_2+\zeta_2^2)(\cos ak + \cos a\epsilon\Big\}, \quad \dots \quad (25)\end{aligned}$$

where

$$S_\pm(k, y, a) = \left(1+\frac{y^2}{4}\right)\cos ak \mp y\cosh\theta \sin a\epsilon \mp \left(1-\frac{y^2}{4}\right)\cos a\epsilon. \qquad \dots \quad (26)$$

$S_+(k, \zeta, a) = 0$ is the dispersion relation for a monatomic lattice. For $\zeta_1 = \zeta_2 = \zeta$, the problem effectively reduces to that of a monatomic lattice with a replaced by $a/2$. An interesting observation may be made from relation (25), that the deviation of the dispersion relation from monatomic lattices, contains a factor $(\zeta_1-\zeta_2)^2$. So that, even if the difference $\zeta_1-\zeta_2$ is not exactly zero but a relatively small quantity, as regards the allowed energy zones, the diatomic lattice behaves like a monatomic lattice with half the lattice distance.

Another important special case which may be of some physical significance, is worth mentioning, the case $\zeta_1 = -\zeta_2$, i.e., the strength of the sources are of same magnitude but alternately changes sign. Expression (24) simply reduces to

$$\left(\frac{1+\zeta^4}{16}\right)(\cos ak-\cos a\epsilon)+\zeta^2\left(\sin^2\frac{ak}{2}-\cosh 2\theta \sin^2\frac{a\epsilon}{2}\right) = 0, \qquad \ldots \quad (27)$$

where $\zeta = |\zeta_1| = |\zeta_2|$. As it is expected from the symmetry of the problem, the dispersion relation depends on ζ^2. Hence, for small ζ, the electronic states are almost those of a free electron except in the neighbourhood of very small kinetic energy of the electron.

References

Fairbairn W. M., Glasser M. L. & Steslicka M. 1973 *Surface Sciences* **36**, 462.
Luttinger J. M. 1951 *Philips Research Report* **6**, 303.
Saxon D. S. & Hunter R. A. 1949 *Philips Research Report* **4**. 81.
Subramanian R. & Bhagwat K. V. 1971 *Phys. Stat. Sol.* **B39**, 399.
——————— 1972 *J. Phys.* **C5**, 798.